Rational Approximation

Qing Yuan*
Central China Normal University, Wuhan 430079, China
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* qyuan@mails.ccnu.edu.cn

I. RATIONAL APPROXIMATION

For a continuous function $f(x)$, we can get its rational approximation $f(x) = \frac{p(x)}{q(x)}$ by using Remez Algorithm. After partial fraction expansion, you get the rational approximation function in the following form:

$$r(x) = \alpha_{const} + \sum_{i=0}^{order-1} \frac{\alpha_i}{x+\beta_i} \tag{1}$$

- Chebyshev's theorem: For any degree (n,d) there is always a unique rational function r that minimises $\|\mathrm{e}\| = \max_{0\leq \mathrm{x}\leq 1}|\mathrm{e(x)}|$, where the error is $e(x) \equiv \frac{r(x)-f(x)}{f(x)}$. In our case, n=d.

- Chebyshev's critierion: The error e(x) takes its maximum absolute value at at least n+d+2 points on the unit interval(which may include the end points of the interval), and the sign of the error alternates between its successive extrema. All the extrema has the same magnitude.

II. THE CONVENTION OF RATIONAL APPROXIMATION IN THE BIELEFELD GPU CODE(CPS CODE)

In Bielefeld GPU code, we want to calculate the following determinant, In the calculation, we need to make rational approximation for it.

$$\left(\frac{\det(M_l^\dagger M_l)}{\det(M_s^\dagger M_s)}\right)^{\frac{1}{2}} (\det M_s^\dagger M_s)^{\frac{3}{4}} = \{\text{psf1}\}\{\text{psf2}\} \tag{2}$$

In this case: $m_s = 0.0591$, $m_l = 0.00591$.

For psf1(light quark):

$$\left(\frac{\det(M_l^\dagger M_l)}{\det(M_s^\dagger M_s)}\right)^{\frac{1}{2}} = \left(\frac{\det(\not{D}^2 + m_l^2)}{\det(\not{D}^2 + m_l^2)}\right)^{\frac{1}{2}} = \det\left(\frac{\not{D}^2 + m_l^2}{\not{D}^2 + m_s^2}\right)^{\frac{1}{2}} \tag{3}$$

The convention used in Bielefeld GPU code is:

$$x = \not{D}^2 + m_l^2 \tag{4}$$

So equation (3) can be rewriten as:

$$\left(\frac{\not{D}^2 + m_l^2}{\not{D}^2 + m_s^2}\right)^{\frac{1}{2}} = \left(\frac{x}{x + m_s^2 - m_l^2}\right)^{\frac{1}{2}} = x^{\frac{1}{2}}(x + m_s^2 - m_l^2)^{-\frac{1}{2}} \tag{5}$$

For psf2(strange quark):

$$(\det M_s^\dagger M_s)^{\frac{3}{4}} = \det(\not{D}^2 + m_s^2)^{\frac{3}{4}} \tag{6}$$

The convention used in Bielefeld GPU code is:

$$x = \not{D}^2 + m_s^2 \tag{7}$$

Inserting it to equation (6), we obtain:

$$(\not{D}^2 + m_s^2)^{\frac{3}{4}} = x^{\frac{3}{4}} \tag{8}$$

The rational approximation will be used by three parts in the RHMC code, they are Heatbath, Acceptance step and Molecular dynamics. Because there two psfs, so you need to generate coefficients for six functions(Each psf need

three functions), they are listed below:
PSF1

$$f(x) = x^{\frac{1}{4}}(x + m_s^2 - m_l^2)^{-\frac{1}{4}} \qquad \text{(for Heatbath)} \tag{9}$$

$$f(x) = x^{-\frac{1}{4}}(x + m_s^2 - m_l^2)^{\frac{1}{4}} \qquad \text{(for acceptance step)} \tag{10}$$

$$f(x) = x^{-\frac{1}{2}}(x + m_s^2 - m_l^2)^{\frac{1}{2}} \qquad \text{(for MD)} \tag{11}$$

PSF2

$$f(x) = x^{\frac{3}{8}} \qquad \text{(for heatbath)} \tag{12}$$

$$f(x) = x^{-\frac{3}{8}} \qquad \text{(for acceptance step)} \tag{13}$$

$$f(x) = x^{-\frac{3}{4}} \qquad \text{(for MD)} \tag{14}$$

I calculate the relative error of function (9) and its rational approximation function to check whether the convention is right. The relative error is defined by equation (15)

$$\mathrm{Err(x)} = \left(\frac{\mathrm{f(x)}}{\mathrm{r(x)}} - 1\right) \times 10^{16} \tag{15}$$

The degree of the rational function is 14. From the figure, you can see the largest error is smaller than 10^{-15}. So we can say our convention is correct.

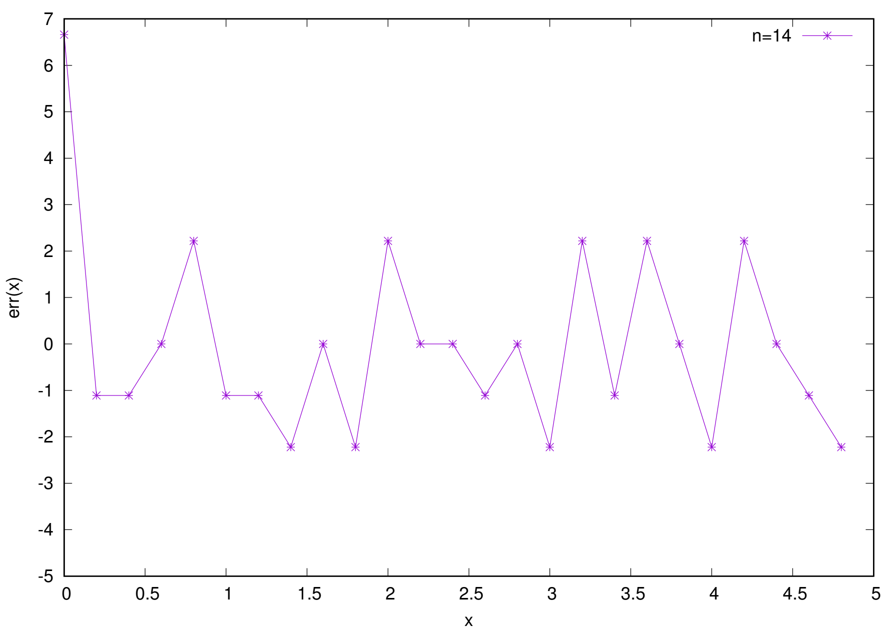

Figure 1. The dependence of Err for light quark (Heatbath) on x. The degree of approximation function is 14.

III. THE CONVENTION OF RATIONAL APPROXIMATION IN THE MILC CODE

The format of the input file of the MILC code is:

1
y_1
y_2
m_2
$order1$
$order2$
λ_{low}
λ_{high}
$precision$

We can generate the coefficients for these following three real functions by using this input file simultaneously

$$f(x) = (x+m_1^2)^{\frac{y_1}{8}}(x+m_2^2)^{\frac{y_2}{8}} \qquad (\mathrm{Heatbath, order1}) \tag{16}$$
$$f(x) = (x+m_1^2)^{-\frac{y_1}{8}}(x+m_2^2)^{-\frac{y_2}{8}} \qquad (\mathrm{acceptance, order1}) \tag{17}$$
$$f(x) = (x+m_1^2)^{-\frac{y_1}{4}}(x+m_2^2)^{-\frac{y_2}{4}} \qquad (\mathrm{MD, order2}) \tag{18}$$

- The parameter “1" in the input file denotes that the number of pseudofermion is one. You can set it to any number you want, but you also need to add additional lines in the input file. Each line represents one pseudofermion.
- The degree of the approximation for Heatbath and acceptance step is order1, the degree of the approximation for Molecular dynamics is order2. λ_{low} and λ_{high} determine the range of x.

IV. RATIONAL APPROXIMATION WITH SIMPLER INPUTS BY USING MILC CODE

We want to generate the coefficients the following six functions which are used in Bielefeld code by using MILC code:

psf1:

$$f(x) = x^{\frac{1}{4}}(x+m_s^2-m_l^2)^{-\frac{1}{4}} \qquad \text{(for Heatbath)} \tag{19}$$
$$f(x) = x^{-\frac{1}{4}}(x+m_s^2-m_l^2)^{\frac{1}{4}} \qquad \text{(for acceptance step)} \tag{20}$$
$$f(x) = x^{-\frac{1}{2}}(x+m_s^2-m_l^2)^{\frac{1}{2}} \qquad \text{(for MD)} \tag{21}$$

psf2:

$$f(x) = x^{\frac{3}{8}} \qquad \text{(for heatbath)} \tag{22}$$
$$f(x) = x^{-\frac{3}{8}} \qquad \text{(for acceptance step)} \tag{23}$$
$$f(x) = x^{-\frac{3}{4}} \qquad \text{(for MD)} \tag{24}$$

We can compare it to the functions which are used in MILC code.

$$f(x) = (x+m_1^2)^{\frac{y_1}{8}}(x+m_2^2)^{\frac{y_2}{8}} \qquad (\mathrm{Heatbath, order1}) \tag{25}$$
$$f(x) = (x+m_1^2)^{-\frac{y_1}{8}}(x+m_2^2)^{-\frac{y_2}{8}} \qquad (\mathrm{acceptance, order1}) \tag{26}$$
$$f(x) = (x+m_1^2)^{-\frac{y_1}{4}}(x+m_2^2)^{-\frac{y_2}{4}} \qquad (\mathrm{MD, order2}) \tag{27}$$

If we want to make the approximation for psf2, We can set the parameters as:

$$\mathrm{y}_1 = 3 \tag{28}$$
$$\mathrm{m}_1 = \mathrm{m}_2 = 0 \tag{29}$$

Other parameters are:

$$\text{order1} = 14 \tag{30}$$
$$\text{order2} = 12 \tag{31}$$
$$\lambda_{low} = m_s^2 = 0.00349281 \tag{32}$$
$$\lambda_{high} = 5.0 \tag{33}$$
$$\text{precision} = 50 \tag{34}$$

If we want to make the approximation for psf1, We can set the parameters as:

$$\mathrm{y}_1 = 2 \tag{35}$$
$$\mathrm{y}_2 = -2 \tag{36}$$
$$\mathrm{m}_2 = (\mathrm{m}_\mathrm{s}^2 - \mathrm{m}_\mathrm{l}^2)^{\frac{1}{2}} = 0.0588037575330012 \tag{37}$$
$$\tag{38}$$

Other parameters are:

$$\text{order1} = 14 \tag{39}$$
$$\text{order2} = 12 \tag{40}$$
$$\lambda_{low} = m_l^2 = 0.0000349281 \tag{41}$$
$$\lambda_{high} = 5.0 \tag{42}$$
$$\text{precision} = 160 \tag{43}$$

So the input file is:

```
2
3
0
0
14
12
0.00349281
5.0
50
2
-2
0.0588037575330012
14
12
0.00003492815
160
```

The second line is parameters for psf2, and the third line is parameters for psf1. The rational function has this form:

$$r(x) = \alpha_{const} + \sum_{i=0}^{order-1} \frac{\alpha_i}{x + \beta_i} \tag{44}$$

Here, order is order1 or order2.

I have ploted the figures of relative error of the real function and rational approximation function using the coefficients generated by Milc code.

$$\mathrm{Err(x)} = \left(\frac{\mathrm{f(x)}}{\mathrm{r(x)}} - 1 \right) \times 10^{16} \tag{45}$$

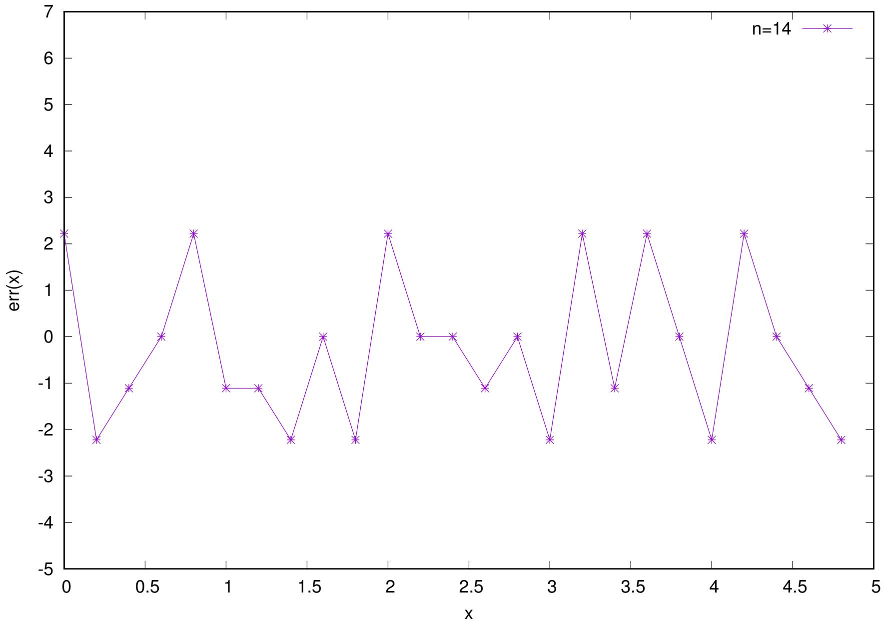

Figure 2. The dependence of Err for light quark (Heatbath) on x. The degree of approximation function is 14.

V. THE DEPENDENCE OF ERR ON THE DEGREE OF APPROXIMATION AND QUARK MASS

Our goal is to find a rational approximation for the following determinant,

$$\left(\frac{\det(M_l^\dagger M_l)}{\det(M_s^\dagger M_s)}\right)^{\frac{1}{2}} (\det M_s^\dagger M_s)^{\frac{3}{4}} = \{\text{psf1}\}\{\text{psf2}\} \tag{46}$$

If we choose different quark mass, the degree of approximation which we need should be different. I choose two different quark masses. In the first case, the heavy quark mass is 0.1138, the light quark mass is 0.004215. The ratio of heavy quark mass and light quark mass is $m_s/m_l = 27$. In the second case, the light quark mass is 0.0009375 and the heavy quark mass is 0.075, the ratio is $m_s/m_l = 80$.
I calculate the maximum relative error(defined by first section) at different degrees of approximation.

For psf2(without hasenbusch), The real function is $f(x) = x^{\frac{3}{8}}$ (heatbath)

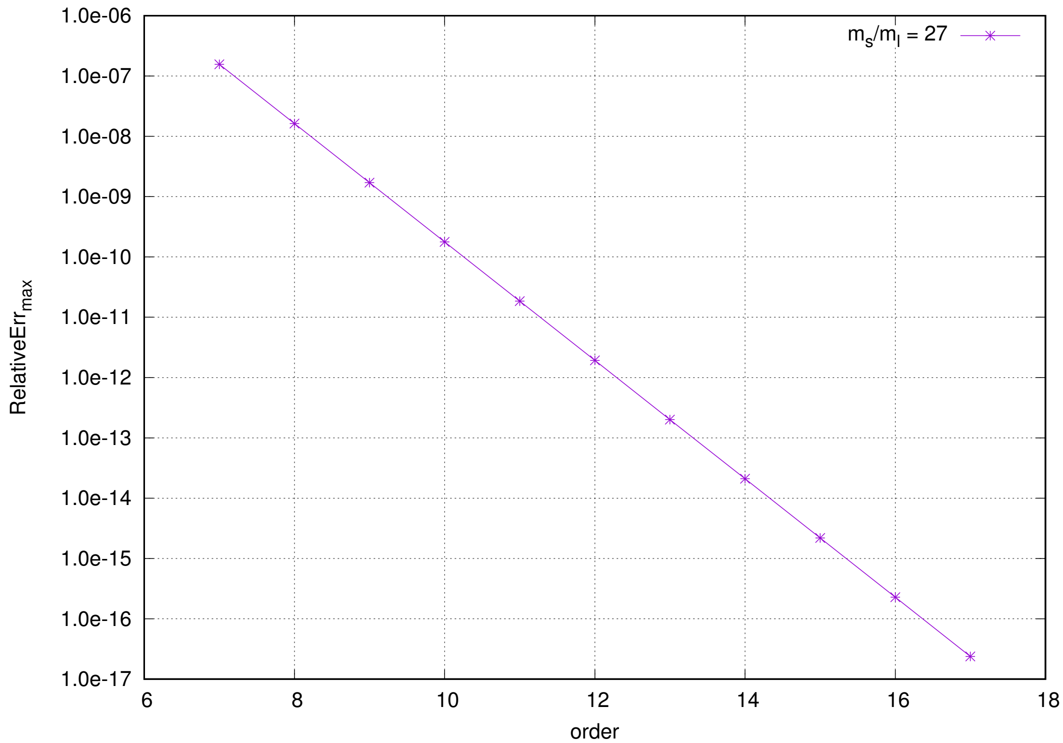

Figure 3. The x axis is degree of approxiamtion and y axis is the maximum relative error. The light quark mass is 0.004215 and heavy quark mass is 0.1138. The precision is 200.

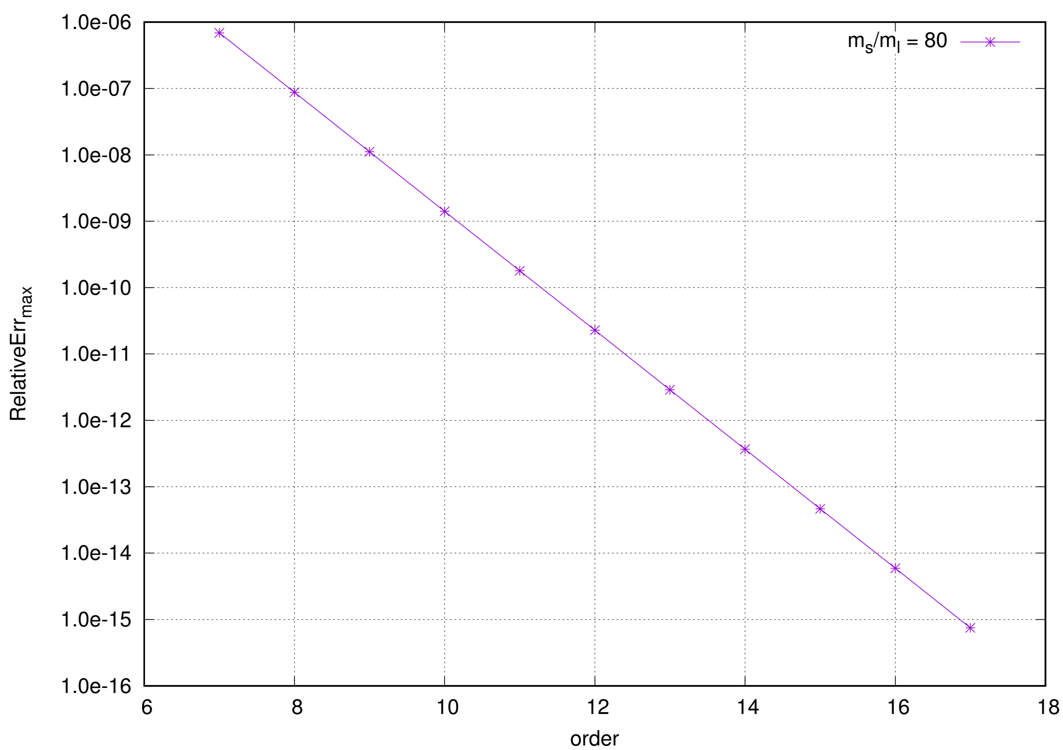

Figure 4. The x axis is degree of approxiamtion and y axis is the maximum relative error. The light quark mass is 0.0009375 and heavy quark mass is 0.075. The precision is 200.

For psf1(with hasenbusch), The real function is $f(x) = x^{\frac{1}{4}}(x + m_s^2 - m_l^2)^{-\frac{1}{4}}$ (heatbath)

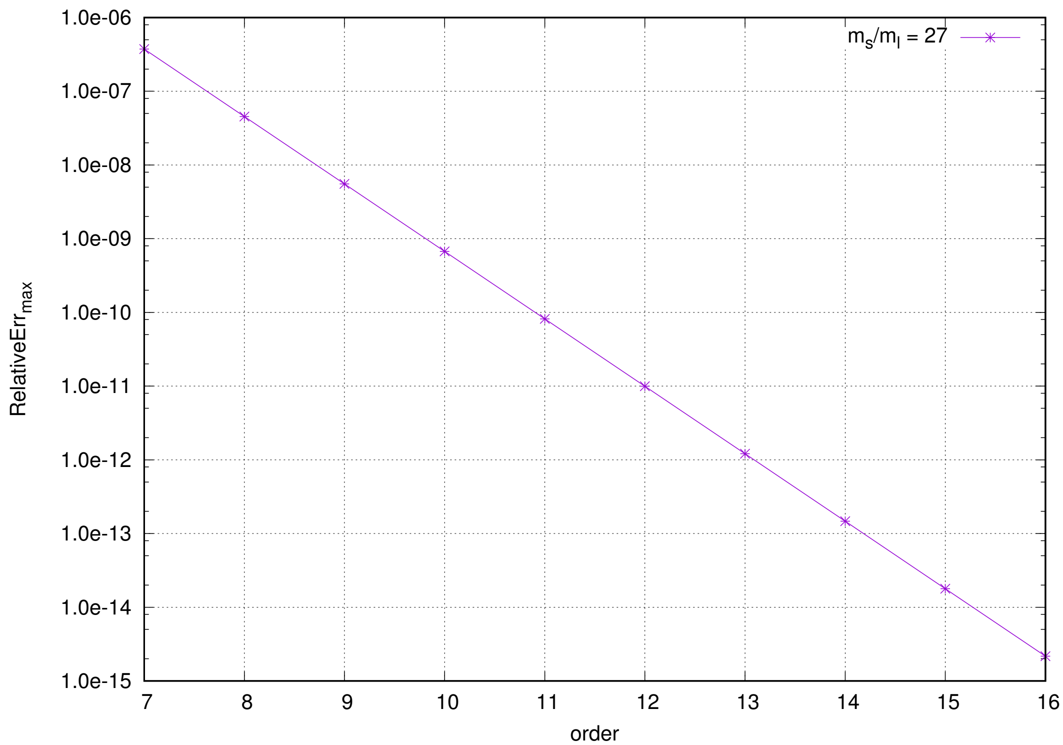

Figure 5. The x axis is degree of approxiamtion and y axis is the maximum relative error. The light quark mass is 0.004215 and heavy quark mass is 0.1138. The precision is 200.

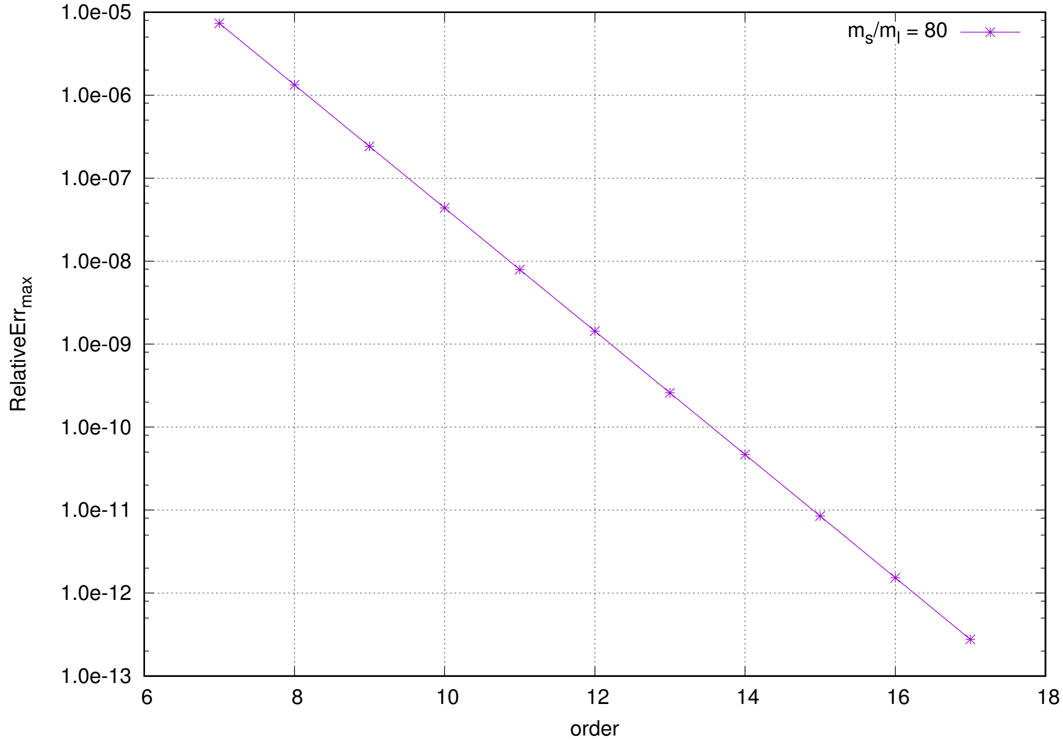

Figure 6. The x axis is degree of approxiamtion and y axis is the maximum relative error. The light quark mass is 0.0009375 and heavy quark mass is 0.075. The precision is 200.

From each of these four figures, we can see if we choose high degrees of approximation, the error will be smaller. And if we compare figure3 and figure4, figure5 and figure6 respectively, we find that for hasenbusch type, if quark mass is small, we need higher degree of approximation to guarantee the relative error is small.

VI. RELATIVE ERROR AT DIFFERENT PRECISION

I calculated the maximum relative error by using different precision. Here the degree of approximation is fixed. From these figures, we can see that the relative maximum error is independent on the precision. But you must set a the precision which should be enough large, otherwish you will not get any results.

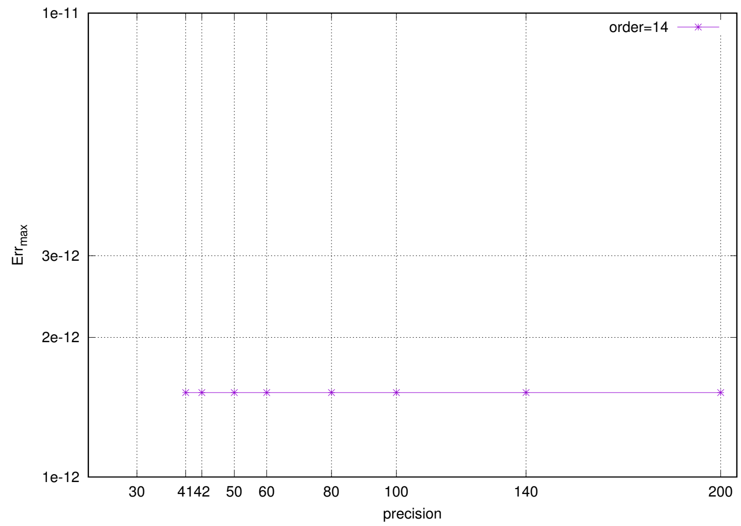

Figure 7. The dependence of Err for light quark(Heatbath) on the precision. Here the degree of approximation is set to be 14.

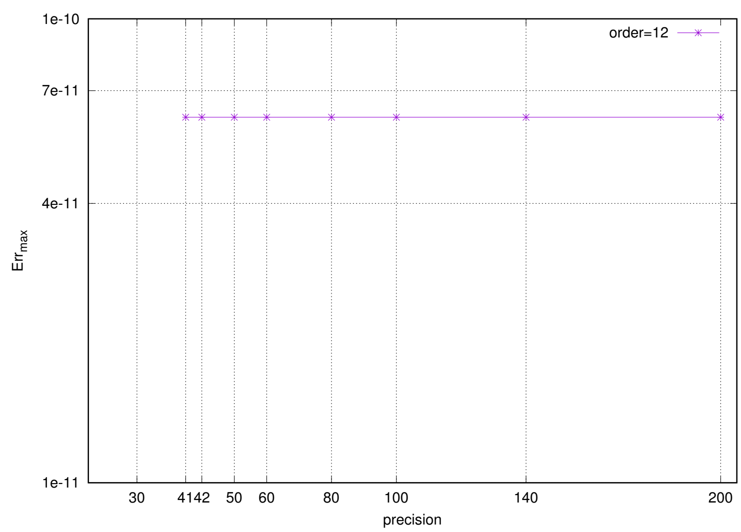

Figure 8. The dependence of Err for light quark(MD) on the precision. Here the degree of approximation is set to be 12.

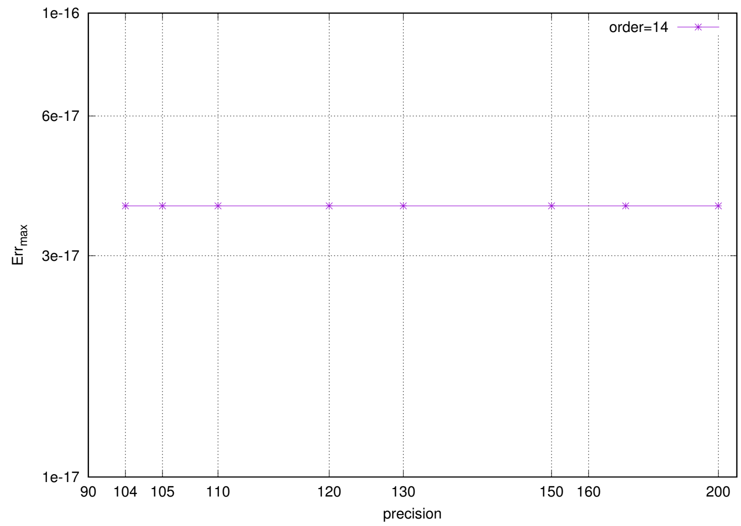

Figure 9. The dependence of Err for strange quark(Heatbath) on the precision. Here the degree of approximation is set to be 14.

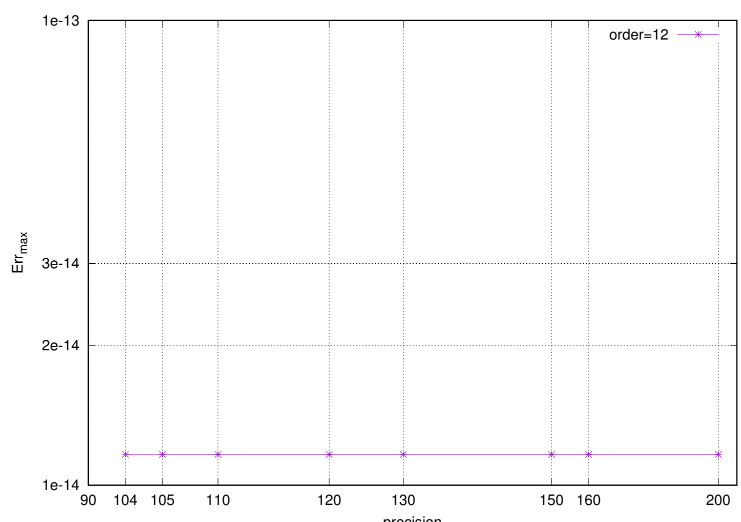

Figure 10. The dependence of Err for strange quark(MD) on the precision. Here the degree of approximation is set to be 12.